

# Effective Hamiltonian, Mori Product and Quantum Dynamics

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An appropriate extension of the effective potential theory is presented that permits the approximate calculation of the dynamical correlation functions for quantum systems. These are obtained by evaluating the generating functionals of the Mori products of quantities related to the relaxation functions in the (PQSCHA) pure self consistent harmonic approximation.

## 1 Dynamic Correlations and Spectral Shapes

The thermodynamics of quantum systems has been widely studied by the effective potential theory<sup>1</sup>: equilibrium properties have been accurately determined<sup>2,3</sup>, but the investigation of dynamical quantities is much more difficult. It is our purpose to give some insights on how the dynamical problem can be approached in terms of the Kubo relaxation functions, that naturally appear in the framework of Mori theory<sup>4</sup>. These functions are obtained by suitably defined scalar products, the Mori products

$$R_{A,B}(t) = (\hat{A}|\hat{B}(t)) = \int_0^{\beta\hbar} du \langle \hat{A}(0) \hat{B}(t + iu) \rangle, \quad (1)$$

where the observables  $\hat{A}$  and  $\hat{B}$  are taken such that  $\langle \hat{A} \rangle = \langle \hat{B} \rangle = 0$ , and braces denote the thermodynamic average. The Laplace transform of Eq.(1) and in particular, the self-relaxation function  $\Xi_0(t) = (\hat{F}_0|\hat{F}_0)^{-1} (\hat{F}_0(t)|\hat{F}_0)$  of an hermitian operator  $\hat{F}_0(t)$  can be Laplace transformed and expanded in a continued fraction, namely  $\Xi_j(z) = (z + \delta_{j+1}\Xi_{j+1}(z))^{-1}$ , where  $\delta_{j+1} = (\hat{F}_j|\hat{F}_j)^{-1} (\hat{F}_{j+1}|\hat{F}_{j+1})$  and  $\hat{F}_j$  denotes the so-called  $j$ -th fluctuating force. The quantities  $(\hat{F}_j|\hat{F}_j)$ , can be related to a combination of the first  $2(j+1)$  moments of the time series-expansion of  $\Xi_0(t)$ . While  $(\hat{F}_j|\hat{F}_j)$  with  $j \neq 0$  can be expressed in terms of static correlations of time derivatives of  $\hat{F}_0$ , the quantity  $(\hat{F}_0|\hat{F}_0)$  requires the direct evaluation of the Mori product.

Indeed, experiments measure the spectral shape, related to  $\Xi_0(z)$  by the “detailed balance” principle:

$$\mathcal{S}(\omega) = (\hat{F}_0 | \hat{F}_0) \frac{\omega}{1 - e^{-\beta\omega}} \frac{1}{\pi} \Re(\Xi_0(z = i\omega)). \quad (2)$$

Therefore,  $\mathcal{S}(\omega)$  can be approached from the knowledge of the static quantities  $\delta_j$  up to a sufficiently large number  $j = J^5$ ,  $\Xi_J(t)^{3,6,5}$ .

## 2 Imaginary-time Ordered Products

Here we shall provide a rigorous derivation of imaginary time ordered products which allows us to control also the evaluation of real time correlators.

We start from the generating functional in the hamiltonian path-integral form:

$$\begin{aligned} Z[L, J] &= \oint \mathcal{D}[x(u)] \int \mathcal{D}[p(u)] \exp[-\frac{1}{\hbar} \mathcal{S}] \\ \mathcal{S} &= \int_0^{\beta\hbar} du \left( -ip(u)\dot{x}(u) + \mathcal{H}(p(u), x(u)) - \hbar L(u)p(u) - \hbar J(u)x(u) \right). \end{aligned} \quad (3)$$

According to the effective potential method<sup>1,3</sup> we use a quadratic trial action. The effective Hamiltonian is  $\mathcal{H}_{\text{eff}}(\eta, \xi) = w(\eta, \xi) + \beta^{-1} \ln(f^{-1} \sinh f)$ , where  $f = \beta\hbar\omega/2$ . By defining the two-component vectors  $\rho = {}^t(\eta, \xi)$  and  $K(u) = {}^t(L(u), J(u))$ , the approximated generating functional can be written as:

$$\begin{aligned} Z_0[K] &= \int \frac{d\eta d\xi}{2\pi\hbar} \exp[-\beta\mathcal{H}_{\text{eff}}(\eta, \xi)] \\ &\cdot \exp\left[ \int_0^{\beta\hbar} du {}^t\rho K(u) + \frac{1}{2} \int_0^{\beta\hbar} du \int_0^{\beta\hbar} dv {}^tK(u) \Phi(u-v) K(v) \right]. \end{aligned} \quad (4)$$

In Eq.(4) we have introduced the  $2 \times 2$  matrix  $\Phi_{k\ell}(u-v)$  with elements  $\Phi_{11}(u-v) = m^2\omega^2 \Phi_{22}(u-v) = m^2\omega^2 \Lambda_f(u-v)$  and  $\Phi_{12}(u-v) = -\Phi_{21}(u-v) = \Gamma_f(u-v)$ , where

$$\begin{aligned} \Lambda_f(u-v) &= \frac{\hbar}{2m\omega \sinh f} \left[ \cosh(|\omega(u-v)| - f) - \frac{\sinh f}{f} \right] \\ \Gamma_f(u-v) &= -\frac{i\hbar \sinh(|\omega(u-v)| - f)}{2 \sinh f} \left[ \theta(u-v) - \theta(v-u) \right]. \end{aligned} \quad (5)$$

While  $\Lambda_f$  is always well defined, the value of  $\Gamma_f$  for  $u = v$  is determined only when the limit  $v - u \rightarrow 0^\pm$  is specified, reflecting the commutation relation of

$\hat{x}$  and  $\hat{p}$  at the same time. Moreover we notice that,  $\Lambda_f(0) = \Lambda_f(\beta\hbar) = \alpha$  and that  $\Lambda_f(u-v)$  and  $\Gamma_f(u-v)$  have a vanishing average in  $[0, \beta\hbar]$ .

Defining the two-component vectors  $\hat{z} = {}^t(\hat{p}, \hat{x})$  and  $y = (y_1(u), y_2(u))$ , the following general formula can be derived<sup>7</sup> in the low-coupling approximation<sup>3</sup>.

$$\left\langle \mathcal{T}_u \left[ \prod_{\nu=1}^N \hat{F}_\nu(\hat{z}_{i_\nu}(u_\nu)) \right] \right\rangle = \mathcal{N} \int \frac{d\eta d\xi}{2\pi\hbar} e^{-\beta\mathcal{H}_{\text{eff}}(\eta, \xi)} \left\langle \left\langle \prod_{\nu=1}^N F_\nu(\rho_{i_\nu} + y_{i_\nu}(u_\nu)) \right\rangle \right\rangle. \quad (6)$$

Where,  $\mathcal{N} = Z_0^{-1}[0]$  is the normalizing factor. The Gaussian average of the variables  $y_{i_\nu}(u_\nu)$  is defined by the second moments

$$\langle \langle y_i(v) y_j(u) \rangle \rangle = \Phi_{ij}(u-v). \quad (7)$$

### 3 Discussion.

The key result<sup>7</sup> is represented by the expression (6), with the definition (7). Indeed, complicated static Mori products, *i.e.* moments of any order, can be evaluated by this last equation. Static correlations can also be obtained performing the appropriate limit  $u-v \rightarrow 0$ .

For instance, when  $(u-v) \rightarrow 0^+$ , we indeed recover our previous result<sup>2,3</sup> for static averages:

$$\langle \hat{A}\hat{B} \rangle = \mathcal{N} \int \frac{d\eta d\xi}{2\pi\hbar} \langle \langle AB \rangle \rangle e^{-\beta\mathcal{H}_{\text{eff}}(\eta, \xi)}, \quad (8)$$

As far as the Mori product is concerned, the well known series expansion  $(2\pi\epsilon)^{-1/2} \exp\{-x^2/(2\epsilon)\} = \sum_{n=0}^{\infty} (1/n!) (\epsilon/2)^n \delta^{(2n)}(x)$  appears to be an efficient tool to approximate the static Mori product of general operators, as well as their dynamical correlations, when the scales of the quantum fluctuations in the system, ruled by  $\hbar$  and the natural length scale  $\alpha$ , are small. It has to be noticed that the averages of  $\Lambda_f(u)$  and  $\Gamma_f(u)$  in  $[0, \beta\hbar]$  are vanishing. An expansion in terms of these quantities has been recently developed<sup>7</sup>.

At the lowest order ( $\hat{A}(p, x)|\hat{B}(p, x)$ ) reduces to the “classical like” average of the product of the Gaussian spreads of the two operators taken at the same order:

$$(\hat{A}(p, x)|\hat{B}(p, x)) = \mathcal{N} \beta\hbar \int \frac{d\eta d\xi}{2\pi\hbar} \langle \langle A(\eta, \xi) \rangle \rangle \langle \langle B(\eta, \xi) \rangle \rangle e^{-\beta\mathcal{H}_{\text{eff}}(\eta, \xi) + o(\alpha, \hbar)}. \quad (9)$$

This zeroth order coincides with the assumption proposed in an attempt<sup>8</sup> to approach also the quantum correlators.

In order to do this, let us notice that harmonic oscillators evolve by the same law both in classical and in quantum dynamics: the differences between quantum and classical statistical evolution are due to the thermal occupation numbers, that are static quantities. Let us suppose that the system evolve with our effective Hamiltonian as found for the thermodynamic behaviour. The Weyl-representation<sup>3</sup> gives us an unified scheme for describing the dynamical variables. The coupling constant  $g$  rules the quantum deviations from the harmonic behaviour and for vanishing  $g$ , Eq.(9) can be assumed to maintain its validity at different real times, provided also that  $\alpha$  is small enough; the result is exact when  $g \rightarrow 0$ . For finite values of  $g$ , the validity of this scheme involves also the amplitudes of the Gaussian fluctuations ruled by the parameter  $\alpha$ . Therefore, there is the same behaviour found for approaching static correlators with the effective Hamiltonian<sup>3</sup>.

At this level, the averages in time of the quantities  $\langle\langle\hat{A}\rangle\rangle$  and  $\langle\langle\hat{B}(t)\rangle\rangle$ , evolving with the effective Hamiltonian  $\mathcal{H}_{\text{eff}}(\xi)$ <sup>8</sup>, can provide an approximation for the time-dependent Mori product  $(\hat{A}|\hat{B}(t))$ .

This procedure yields a good approximation for times up to the order of  $\hbar\beta$ , for which the use of the effective potential makes sense in the calculation of the static quantities at lowest order, reproducing for instance a correct second moment for the displacement-displacement dynamic correlator with a well-behaved classical long time decay.

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